Acetic acid, trifluoro-, methyl ester

431-47-0 | DTXSID2059988

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 4.99 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.30e-01

Confidence level: 8.45e-01

Nearest Neighbors from the Training Set

Image not found
Dalapon
Measured: 2.51
Predicted: 2.04

Image not found
Dalapon-sodium
Measured: 1.00
Predicted: 2.04

Image not found
Epichlorohydrin
Measured: 10.0
Predicted: 9.87

Image not found
3-Pyridinecarbonitrile
Measured: 36.3
Predicted: 25.0

Image not found
Methyl isothiocyanate
Measured: 9.33
Predicted: 7.63